6-(2-Methylbutyryloxy)-hyoscyamine

Inchi: InChI=1S/C22H31NO5/c1-4-14(2)21(25)28-20-11-16-10-17(12-19(20)23(16)3)27-22(26)1
InchiKey: ATYKKAWWFYYZJF-QHGFLKOESA-N
Formula: C22H31NO5
SMILES: CCC(C)C(=O)OC1CC2CC(OC(=O)C(CO)c3ccccc3)CC1N2C
Mol. weight [g/mol]: 389.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.499		Crippen Method
mcvol	306.090	ml/mol	McGowan Method
rinpol	2539.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R421720&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices